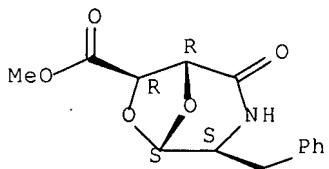


ST1C Search

RN 250138-10-4 CAPLUS

CN 6,8-Dioxa-3-azabicyclo[3.2.1]octane-7-carboxylic acid,
2-oxo-4-(phenylmethyl)-, methyl ester, (1R,4S,5S,7R)- (CA INDEX NAME)

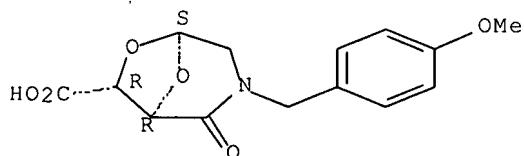
Absolute stereochemistry. Rotation (-).



RN 250138-20-6 CAPLUS

CN 6,8-Dioxa-3-azabicyclo[3.2.1]octane-7-carboxylic acid,
3-[(4-methoxyphenyl)methyl]-2-oxo-, (1R,5S,7R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L14 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1999:580083 CAPLUS Full-text

DOCUMENT NUMBER: 131:337331

TITLE: Synthesis and Reactivity of Bicycles Derived from
Tartaric Acid and α -Amino Acids: A Novel Class
of Conformationally Constrained Dipeptide Isosteres
Based upon Enantiopure 3-Aza-6,8-dioxabicyclo[3.2.1]octane-7-carboxylic Acid
Guarna, Antonio; Guidi, Antonio; Machetti,

Fabrizio; Menchi, Gloria; Occhiato, Ernesto G.;

Scarpi, Dina; Sisi, Sauro; Trabocchi, Andrea

AUTHOR(S): Department of Organic Chemistry U. Schiff and Center
of Heterocyclic Compounds C.N.R., University of
Florence, Florence, I-50121, ItalyCORPORATE SOURCE: Journal of Organic Chemistry (1999), 64(20), 7347-7364
SOURCE: CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

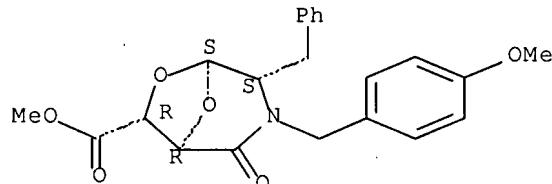
OTHER SOURCE(S): CASREACT 131:337331

AB 3-Aza-6,8-dioxabicyclo[3.2.1]octane-7-carboxylic acids (named BTAA) derived from (R,R)-, (S,S)-, or meso-tartaric acid and natural (L), unnatural (D), or unusual α -amino acids are described as conformationally constrained dipeptide isosteres. The general strategy developed for their preparation has required the transformation of the amino acids into the corresponding N-benzyl-amino alcs., followed by the PyBroP-promoted condensation with the monomethyl ester of the suitable 2,3-di-O-isopropylidene-tartaric acid. Oxidation of the hydroxy group to aldehyde and subsequent acid-catalyzed trans-acetalization with the two hydroxy groups of the tartaric acid moiety provided 3-aza-2-oxo-6,8-dioxabicyclo[3.2.1]octane-7-carboxylic acid Me esters [named BTAA(O)] in good yield and, in most cases, as single enantiopure diastereoisomers. This strategy has been applied to the preparation of BTAA(O) starting from (R,R)-, (S,S)-, or meso-tartaric acid and glycine, L- and D-phenylalanine, L- and D-alanine, and (\pm)-phenylglycine. In the cases of glycine, L- and D-phenylalanine, and L- and D-alanine, the selective reduction by BH₃·DMS of the amide group succeeding to the cyclization step, or the reduction of both amide and ester functions followed by reoxidn. of the hydroxy to carboxylic group, provided in good yield the 3-aza-3-benzyl-6,8-dioxabicyclo[3.2.1]octane-7-carboxylic acids (or their Me ester) BTAA, having the side chain of the amino acid precursors at position 4. The stability and rigidity of the bicyclic skeleton, the complete control of all the stereo-centers, the possibility of introducing the side chains of L- or D-amino acids, and the demonstrated compatibility with the conditions required for solid-phase peptide synthesis make the BTAA compds. potential dipeptide isosteres useful for the synthesis of modified peptides.

IT 198978-51-7P 250137-79-2P 250137-80-5P
 250137-81-6P 250137-82-7P 250137-84-9P
 250137-85-0P 250137-86-1P 250137-87-2P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and reaction of in the synthesis of 3-aza-6,8-dioxabicyclo[3.2.1]octane-7-carboxylic acid as conformationally constrained dipeptide isosteres)

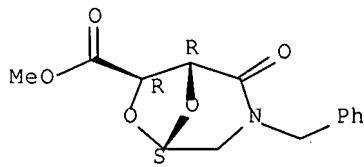
RN 198978-51-7 CAPLUS
 CN 6,8-Dioxa-3-azabicyclo[3.2.1]octane-7-carboxylic acid,
 3-[(4-methoxyphenyl)methyl]-2-oxo-4-(phenylmethyl)-, methyl ester,
 (1R,4S,5S,7R)- (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 250137-79-2 CAPLUS
 CN 6,8-Dioxa-3-azabicyclo[3.2.1]octane-7-carboxylic acid,
 2-oxo-3-(phenylmethyl)-, methyl ester, (1R,5S,7R)- (CA INDEX NAME)

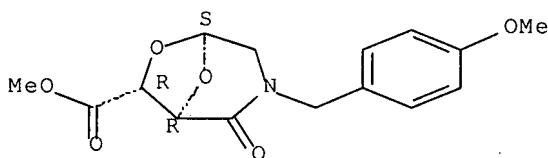
Absolute stereochemistry. Rotation (-).



RN 250137-80-5 CAPLUS

CN 6,8-Dioxa-3-azabicyclo[3.2.1]octane-7-carboxylic acid,
3-[(4-methoxyphenyl)methyl]-2-oxo-, methyl ester, (1R,5S,7R)- (CA INDEX
NAME)

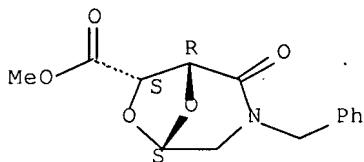
Absolute stereochemistry. Rotation (-).



RN 250137-81-6 CAPLUS

CN 6,8-Dioxa-3-azabicyclo[3.2.1]octane-7-carboxylic acid,
2-oxo-3-(phenylmethyl)-, methyl ester, (1R,5S,7S)-rel- (CA INDEX NAME)

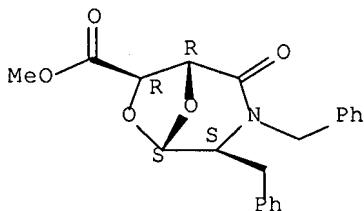
Relative stereochemistry.



RN 250137-82-7 CAPLUS

CN 6,8-Dioxa-3-azabicyclo[3.2.1]octane-7-carboxylic acid,
2-oxo-3,4-bis(phenylmethyl)-, methyl ester, (1R,4S,5S,7R)- (CA INDEX
NAME)

Absolute stereochemistry. Rotation (-).

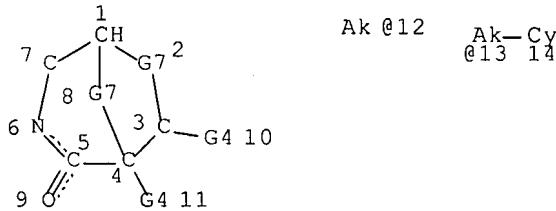


RN 250137-84-9 CAPLUS

CN 6,8-Dioxa-3-azabicyclo[3.2.1]octane-7-carboxylic acid,

SEARCH HISTORY

=> d stat que 112; d his nofile
L9 STR



Ak @12 Ak-Cy
@13 14

VAR G4=H/12/CY/13

VAR G7=O/S/N

NODE ATTRIBUTES:

CONNECT IS E1 RC AT 12
CONNECT IS E2 RC AT 13
DEFAULT MLEVEL IS ATOM
MLEVEL IS CLASS AT 12 13 14
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC 1

NUMBER OF NODES IS 14

STEREO ATTRIBUTES: NONE

L12 225 SEA FILE=REGISTRY SSS FUL L9

100.0% PROCESSED 44361 ITERATIONS

225 ANSWERS

SEARCH TIME: 00.00.03

(FILE 'HOME' ENTERED AT 10:51:09 ON 13 NOV 2007)

FILE 'CAPLUS' ENTERED AT 10:51:55 ON 13 NOV 2007
E US2004-518689/APPS

L1 1 SEA ABB=ON US2004-518689/AP
D SCAN
L2 140 SEA ABB=ON GUARNA A?/AU
L3 41 SEA ABB=ON COZZOLINO F?/AU
L4 21 SEA ABB=ON TORCIA M?/AU
L5 235 SEA ABB=ON GARACI E?/AU

FILE 'REGISTRY' ENTERED AT 10:52:49 ON 13 NOV 2007

L6 STR
L7 7 SEA SSS SAM L6

FILE 'ZCAPLUS' ENTERED AT 10:57:02 ON 13 NOV 2007
L8 7 SEA ABB=ON L7

FILE 'REGISTRY' ENTERED AT 10:57:13 ON 13 NOV 2007
L9 STR L6
L10 6 SEA SSS SAM L9
L11 44361 SEA SSS FUL L9 EXTEND

L12 225 SEA SSS FUL L9

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L13 38 SEA ABB=ON L12
L14 11 SEA ABB=ON (L1 OR L2 OR L3 OR L4 OR L5) AND L13
L15 1 SEA ABB=ON L1 AND L13

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D QUE NOS L14
D IBIB ABS HITSTR L14 1-11

FILE 'REGISTRY' ENTERED AT 11:00:44 ON 13 NOV 2007
D STAT QUE L12

FILE 'CAPPLUS' ENTERED AT 11:00:44 ON 13 NOV 2007
D QUE NOS L13
L16 27 SEA ABB=ON L13 NOT L14
D IBIB ABS HITSTR L16 1-27

FILE 'HOME' ENTERED AT 11:01:07 ON 13 NOV 2007
D STAT QUE L12

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